10,11-Dihydro-5H-dibenz(b,f)azepin-5-amine
7458-07-3 | DTXSID00225559

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 127 °C

Global applicability domain: Inside

Local applicability domain index: 4.47e-01

Confidence level: 3.49e-01

Nearest Neighbors from the Training Set

Image not found
1,1-Diphenylhydrazine
Measured: 50.5
Predicted: 72.2

Image not found
Methanone, diphenyl-, hydrazone
Measured: 96.5
Predicted: 99.1

Image not found
2-Phenylbenzimidazole
Measured: 293
Predicted: 195

Image not found
1-Naphthalenecarbonitrile, 4-amino-
Measured: 176
Predicted: 153